Journal of Molecular Structure (Theochem), 257 (1992) 509
Elsevier Science Publishers B.V., Amsterdam

AUTHOR INDEX

Adamowicz, L., 491

Bencivenni, L., 369
Bergson, G., 325
Bodor, N., 49
Boucekkine, A., 175
Brewster, M.E., 49
Buemmi, G., 243

Caminiti, L., 369
Carlsen, P.H.J., 105, 131
Castro, E.A., 205
Cheam, T.C., 57
Chung-Phillips, A., 417

Dantas, S.O., 437
De Almeida, W.B., 305

Eriksson, L.A., 325
Euler, W.B., 227

Feltrin, A., 369
Ferris, K.F., 499
Fu, X.Y., 25

Galasso, V., 181
Galvão, D.S. 437
Garcia, Mª J.R., 279
Guha, S., 451

Hadži, D., 475
Hansen, P., 75
Harb, V., 475
Hong, S.G., 25
Huang, M.-J., 49
Huelmo, J. Mª H, 279

Jayasuriya, K., 405
Jhon, M.S., 33
Jubert, A.H., 205

Keese, R., 353
Koča, J., 105, 131
Kocjan, D., 475
Kwiatkowski, J.S., 85

Lai, W.J., 217
Lés, A., 491
Leszczynski, J., 85
Li, W.-K., 189
Lin, Y., 167
Luef, W., 353

Majumbar, D., 451
Meghezzi, H., 175
Meyer, M., 157

Öhrn, N.Y., 325
Ottavianelli, E.E., 205
O'Malley, P.J., 305

Palofax, M.A., 259
Pang, L., 143

Qu, X., 25

Ramondo, F., 369
Riggs, N.V., 189
Russo, N., 485

Sadun, C., 369
Schmitz, B.K., 227
Sicilia, E., 485
Slanina, Z., 491
Song, M.Y., 33
Steiger, T., 313
Stepanov, A.V., 1
Steudal, R., 313

Tavgin, V.L., 1
Toscano, M., 485

Whitehead, M.A., 143

Yilmaz, H., 285

Zhang, F., 167
Zheng, M., 75

Journal of Molecular Structure (Theochem), 257 (1992) 511–513
Elsevier Science Publishers B.V., Amsterdam

SUBJECT INDEX

(4-Aminophenyl)borane
Semiempirical MO study of charge transfer in (4-aminophenyl)borane and related compounds: molecular "paddle-wheels," 325

Benzenoid systems
An algorithm for recognizing Kekulé structures in benzenoid and coronoid systems, 167

$C_3H_3^+$
An ab initio molecular orbital study of the $C_3H_3^+$ potential energy surface, 189

C≡P group
A computational investigation of the effects of substituents on the C≡P group, 405

Carboxylic acids
Geometries and vibrational frequencies of oxyacids and carboxylic acids. A study on structural and vibrational effects, 369

CCl_3Z (Z=H,F,Cl,Br,I,CH_3,CF_3,CN or NO_2)
Computational investigation of the molecular orientation and dynamics of CCl_3Z guest molecules in clathrates of Dianin's compound and its mercapto analogue, 143

CF_3OOX (X=H,F,Cl)
Ab initio study of the electronic, vibrational and rotational properties of CF_3OOX (X=H,F,Cl), 205

$(CH_3)_2CHX$ (X=H,F,Cl)
Comparative ab initio study of $(CH_3)_2CHX$ (X=F,Cl) and $(CH_3)_2CX_2$-type molecules (X=H,F,Cl), 157

$(CH_3)_2CX_2$ (X=H,F,Cl)
Comparative ab initio study of $(CH_3)_2CHX$ (X=F,Cl) and $(CH_3)_2CX_2$-type molecules (X=H,F,Cl), 157

Coronoid systems
An algorithm for recognizing Kekulé structures in benzenoid and coronoid systems, 167

Covalent crystals
Activation model: application for diffusivity in covalent crystals, 1

CuO–ZnO catalysts
Quantum chemistry study on the nature of the CO and H_2 activation of CuO–ZnO catalysts for methanol synthesis, 217

DAISY
DAISY, a computational method: a novel tool for the study of the conformational behavior of flexible molecules, 105

Dianin's compound
Computational investigation of the molecular orientation and dynamics of CCl_3Z guest molecules in clathrates of Dianin's compound and its mercapto analogue, 143

Diazabicycloanols
Conformational study of several diazabicycloanols by the AM1 method, 259

Dithioacetylacetone
Ab initio study of the thioketo–enethiol tautomerism of dithiomalondialdehyde and dithioacetylacetone, 243

Dithiomalondialdehyde
Ab initio study of the thioketo–enethiol tautomerism of dithiomalondialdehyde and dithioacetylacetone, 243

DNA
Molecular dynamics study of the effect of ion concentration on the B-DNA, Z-DNA and DNA-daunomycin complex, 33

DNA-daunomycin complex
Molecular dynamics study of the effect of ion concentration on the B-DNA, Z-DNA and DNA-daunomycin complex, 33

Ellipticine
An investigation of the electronic structure of the antitumour drug ellipticine and its derivatives. Part II. Spectroscopic INDO/CI study, 437

Ethane-1,2-dithiol
Conformation and structure of ethane-1,2-dithiol from ab initio HF and MP3 study, 485

Fulvalenes
A Green's function ab initio study of the outer valence ionization potentials of the simplest fulvenes, fulvalenes and spirenes, 181

Fulvenes
A Green's function ab initio study of the outer valence ionization potentials of the simplest fulvenes, fulvalenes and spirenes, 181

GABA mediators
Effect of hydration on the conformational properties and pharmacophoric pattern of several GABA mediators, 451

$H_4ALO_4^-$
Ab initio molecular orbital calculated stationary points on the potential energy surface of $H_4AlO_4^-$ — similarities with H_4SiO_4, 305

H_4SiO_4
Ab initio molecular orbital calculated stationary points on the potential energy surface of $H_4AlO_4^-$ — similarities with H_4SiO_4, 305

HCN oligomerization
A quantum chemical study of the mechanism of HCN oligomerization, 25

Hexagonal systems
A linear algorithm for fixed bonds in hexagonal systems, 75

Hydrazine
A comparative theoretical study of hydrazine, 227

Hydroxypyrones
Influence of the entropic terms on the tautomeric equilibria of hydroxypyrones, 175

Internal rotation
An ab initio study of internal rotation, 417

Metacyclophanes
Theoretical study using the AM1 method of the metacyclophanes *anti*-[2.2]metacyclophane-1,9-diene, dihydropyrene, and pyrene, 279

Methanol
Quantum chemistry study on the nature of the CO and H_2 activation of CuO–ZnO catalysts for methanol synthesis, 217

Methylacetamide
Ab initio vibrational spectra of hydrogen-bonded *N*-methylacetamide, 57

Organophosphorus compounds
The quantitative prediction and interpretation of vibrational spectra of organophosphorus compounds. Part III. Comparative ab initio SCF studies of phosphine oxide, phosphine sulfide and their fluoroderivatives, 85

Orthosilic acid
SCF and correlated level determination of the molecular and vibrational structure of orthosilic acid, $Si(OH)_4$, 499

Oxyacids
Geometries and vibrational frequencies of oxyacids and carboxylic acids. A study on structural and vibrational effects, 369

Phosphorus
Structural stability and energetics of the

phosphorus microclusters P_2 to P_{10}: and MNDO calculation, 285

Pyridines
Reactivity of biologically important reduced pyridines. Part 9. Effect of substitution on rotational energetics in 1-phenyl-1,4-dihydropyridine, the 1-phenylpyridinium cation and related systems, 49

Pyridone/hydroxypyridine
Dimerization in the pyridone/hydroxypyridine tautomeric systems: relative stabilities of the dimers in the 2-pyridone/2-hydroxypyridine and in the 4-pyridine/4-hydroxypyridine systems, 491

Quinolone analogues
A comparative semiempirical and ab initio study of tautomerization energies. 7-Methyl-2,3,4,7-tetrahydroisothiazolo-[5,4b]pyridine-3,4-dione and other models of antibacterial quinolone analogues, 475

ROSE
ROSE, a computer program for automatic generation of probable conformations, 131

Spirenes
A Green's function ab initio study of the outer valence ionization potentials of the simplest fulvenes, fulvalenes and spirenes, 181

Spiroalkanes
Angular distortions at tetracoordinate carbon: planoid distortions in small spiroalkanes, 353

Sulphoxylic acid
Sulphur compounds. Part 149. Structures, relative stabilities and vibrational spectra of several isomeric forms of sulphoxylic acid (H_2SO_2) and its anion (HSO_2^-): ab initio study, 313